

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG020223\
 Data File : BG056530.D
 Acq On : 3 Feb 2023 1:41
 Operator : CG/JU
 Sample : 01401-01 10X
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 OK-1-212023

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG012723.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG056530.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.309	340	344	352	rBB3	7381	11926	1.59%	0.179%
2	5.802	421	428	437	rBB	28559	49754	6.65%	0.746%
3	7.424	697	704	712	rBV	31653	54233	7.25%	0.813%
4	8.276	843	849	858	rVB	148617	258253	34.50%	3.872%
5	9.457	1042	1050	1055	rBV	19445	40698	5.44%	0.610%
6	10.285	1185	1191	1197	rBV5	5372	8077	1.08%	0.121%
7	10.497	1223	1227	1232	rBV3	7129	11921	1.59%	0.179%
8	11.049	1314	1321	1324	rBV2	12507	20692	2.76%	0.310%
9	11.114	1324	1332	1340	rVB	194686	355992	47.56%	5.337%
10	11.231	1345	1352	1357	rVB5	7351	14987	2.00%	0.225%
11	11.578	1407	1411	1416	rVB4	4554	7881	1.05%	0.118%
12	11.789	1439	1447	1453	rBV9	7130	15140	2.02%	0.227%
13	11.924	1463	1470	1475	rVB7	6042	11907	1.59%	0.179%
14	12.007	1481	1484	1489	rVB4	5548	8278	1.11%	0.124%
15	12.083	1493	1497	1502	rVB6	6324	11230	1.50%	0.168%
16	12.136	1502	1506	1512	rVB5	5046	7592	1.01%	0.114%
17	12.283	1523	1531	1537	rBV2	16690	29382	3.93%	0.440%
18	12.471	1558	1563	1572	rBV3	20538	33895	4.53%	0.508%
19	12.982	1642	1650	1656	rBV5	15145	27145	3.63%	0.407%
20	13.241	1690	1694	1696	rBV4	6968	10201	1.36%	0.153%
21	13.411	1717	1723	1726	rBV4	10901	15501	2.07%	0.232%
22	13.523	1736	1742	1752	rVB	84194	131024	17.50%	1.964%
23	13.693	1766	1771	1777	rVB2	30359	43065	5.75%	0.646%
24	13.840	1790	1796	1801	rVB6	10974	20615	2.75%	0.309%
25	14.169	1847	1852	1856	rBV5	8049	15741	2.10%	0.236%
26	14.216	1856	1860	1864	rVV7	11596	19352	2.59%	0.290%
27	14.257	1864	1867	1874	rVV9	10663	20876	2.79%	0.313%
28	14.322	1874	1878	1879	rVV3	12625	15951	2.13%	0.239%
29	14.345	1879	1882	1886	rVV4	19172	26838	3.59%	0.402%
30	14.398	1886	1891	1895	rVV7	11509	21986	2.94%	0.330%
31	14.463	1895	1902	1907	rVV8	11958	22231	2.97%	0.333%
32	14.545	1912	1916	1921	rVB7	5228	8354	1.12%	0.125%
33	14.639	1928	1932	1938	rVB8	5315	9046	1.21%	0.136%
34	14.751	1947	1951	1958	rVB	37047	54144	7.23%	0.812%
35	14.897	1967	1976	1984	rVB	343703	544403	72.73%	8.161%
36	15.027	1994	1998	2001	rVB5	5700	8537	1.14%	0.128%

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Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG012723.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.097	2005	2010	2014	rBV6	8202	15659	2.09%	0.235%
38	15.244	2032	2035	2039	rVV6	7480	10918	1.46%	0.164%
39	15.291	2039	2043	2051	rVB8	8140	17462	2.33%	0.262%
40	15.367	2051	2056	2060	rBV6	13409	25519	3.41%	0.383%

41	15.432	2064	2067	2072	rVB6	8133	12629	1.69%	0.189%
42	15.503	2074	2079	2082	rBV6	10155	19745	2.64%	0.296%
43	15.696	2105	2112	2116	rBV	48959	65848	8.80%	0.987%
44	15.808	2126	2131	2133	rBV4	5602	7854	1.05%	0.118%
45	15.914	2143	2149	2150	rBV5	4709	7880	1.05%	0.118%

46	16.096	2172	2180	2185	rBV7	21887	50920	6.80%	0.763%
47	16.196	2193	2197	2201	rBV6	9823	12153	1.62%	0.182%
48	16.313	2215	2217	2223	rVB7	7876	11727	1.57%	0.176%
49	16.378	2223	2228	2235	rBV2	47430	75195	10.05%	1.127%
50	16.554	2254	2258	2261	rBV	49616	71871	9.60%	1.077%

51	16.895	2313	2316	2320	rBV5	7345	10318	1.38%	0.155%
52	17.065	2342	2345	2350	rVB5	10405	13961	1.87%	0.209%
53	17.130	2352	2356	2359	rBV5	6163	8572	1.15%	0.129%
54	17.347	2388	2393	2397	rVB	45014	52570	7.02%	0.788%
55	17.400	2398	2402	2407	rVB5	19069	24591	3.29%	0.369%

56	17.635	2436	2442	2448	rBV	435666	662558	88.52%	9.933%
57	17.677	2448	2449	2454	rVB	21810	21301	2.85%	0.319%
58	17.776	2463	2466	2469	rVB5	7089	7866	1.05%	0.118%
59	17.818	2471	2473	2480	rVB8	7365	11843	1.58%	0.178%
60	17.953	2494	2496	2500	rBV4	6131	8573	1.15%	0.129%

61	18.082	2515	2518	2523	rVV	42609	58574	7.83%	0.878%
62	18.135	2523	2527	2531	rVB7	14258	20292	2.71%	0.304%
63	18.258	2543	2548	2555	rVB	199744	247487	33.06%	3.710%
64	18.352	2560	2564	2569	rBV7	11343	22163	2.96%	0.332%
65	18.487	2583	2587	2590	rBV4	24122	36923	4.93%	0.554%

66	18.687	2617	2621	2622	rBV4	13049	13155	1.76%	0.197%
67	18.769	2631	2635	2639	rVB	42983	53059	7.09%	0.795%
68	19.292	2720	2724	2727	rBV6	10749	14566	1.95%	0.218%
69	19.386	2735	2740	2742	rBV2	354214	445907	59.57%	6.685%
70	19.416	2742	2745	2749	rVB	479316	550583	73.56%	8.254%

71	19.539	2763	2766	2771	rBV	102519	134692	17.99%	2.019%
72	19.604	2774	2777	2778	rVV3	28939	35013	4.68%	0.525%
73	19.627	2778	2781	2784	rVV4	44582	66264	8.85%	0.993%
74	19.674	2786	2789	2794	rVB	32724	50346	6.73%	0.755%
75	19.903	2826	2828	2831	rBV4	17133	17182	2.30%	0.258%

76	19.956	2835	2837	2841	rVB	33088	31855	4.26%	0.478%
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ClientSampleId :
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Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG012723.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

77	20.033	2847	2850	2857	rVB	42747	64722	8.65%	0.970%
78	20.209	2876	2880	2885	rVB	148019	186304	24.89%	2.793%
79	21.930	3167	3173	3184	rVB	433733	748522	100.00%	11.221%
80	25.362	3751	3757	3769	rVB	237548	678549	90.65%	10.172%

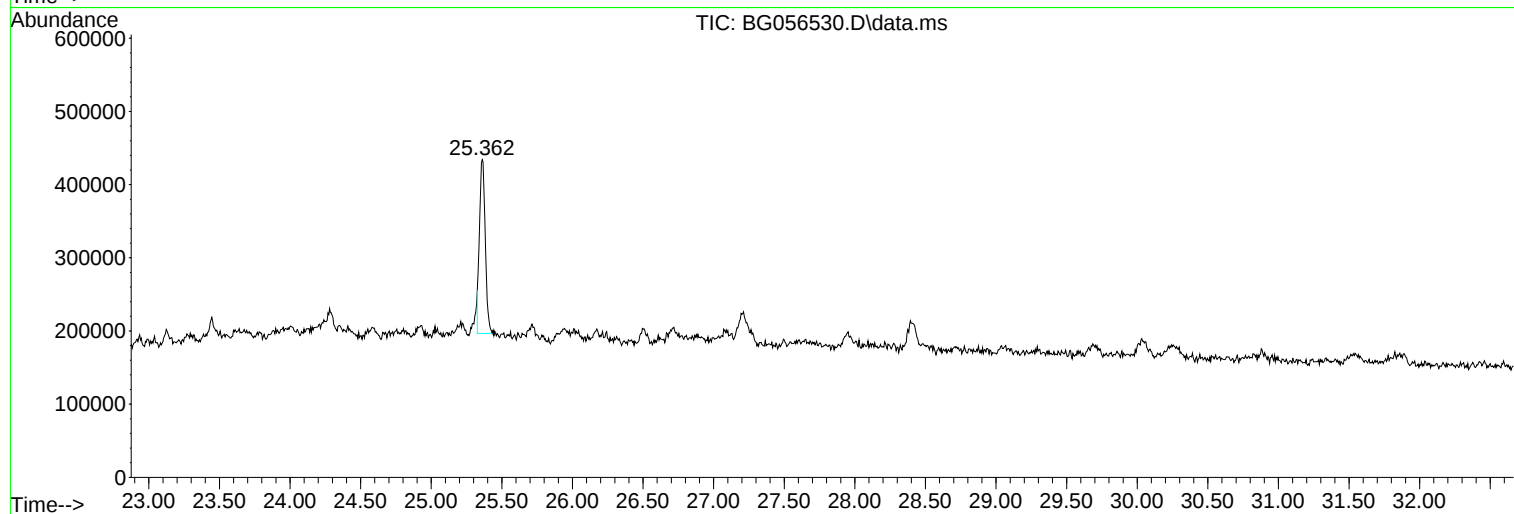
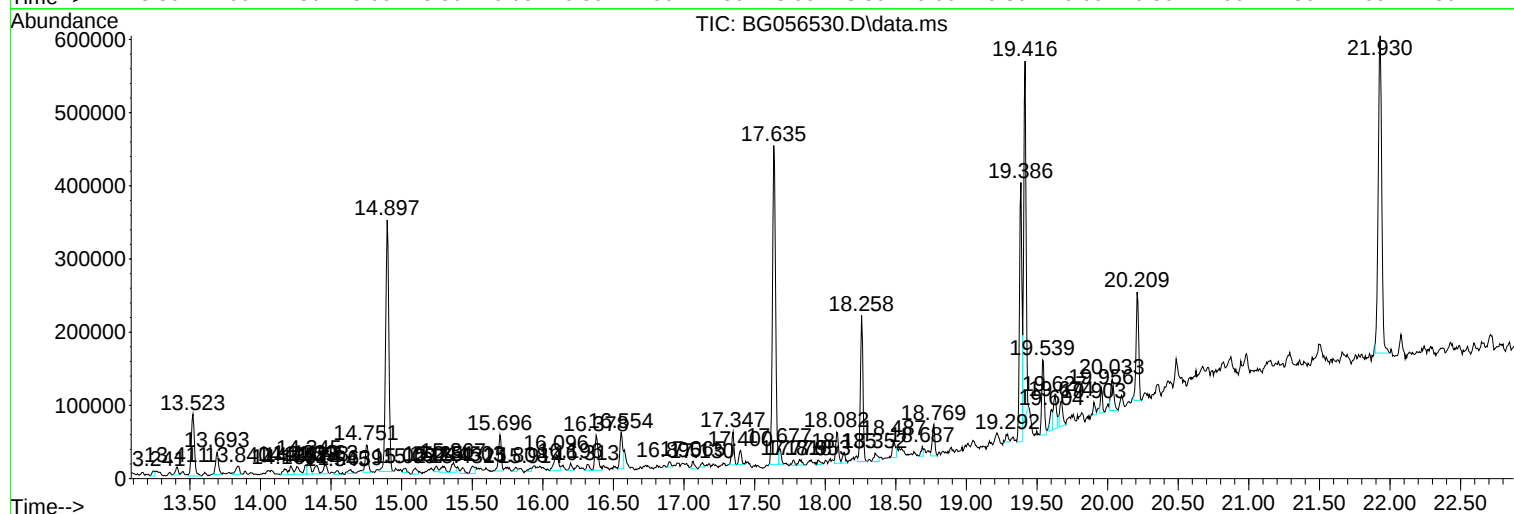
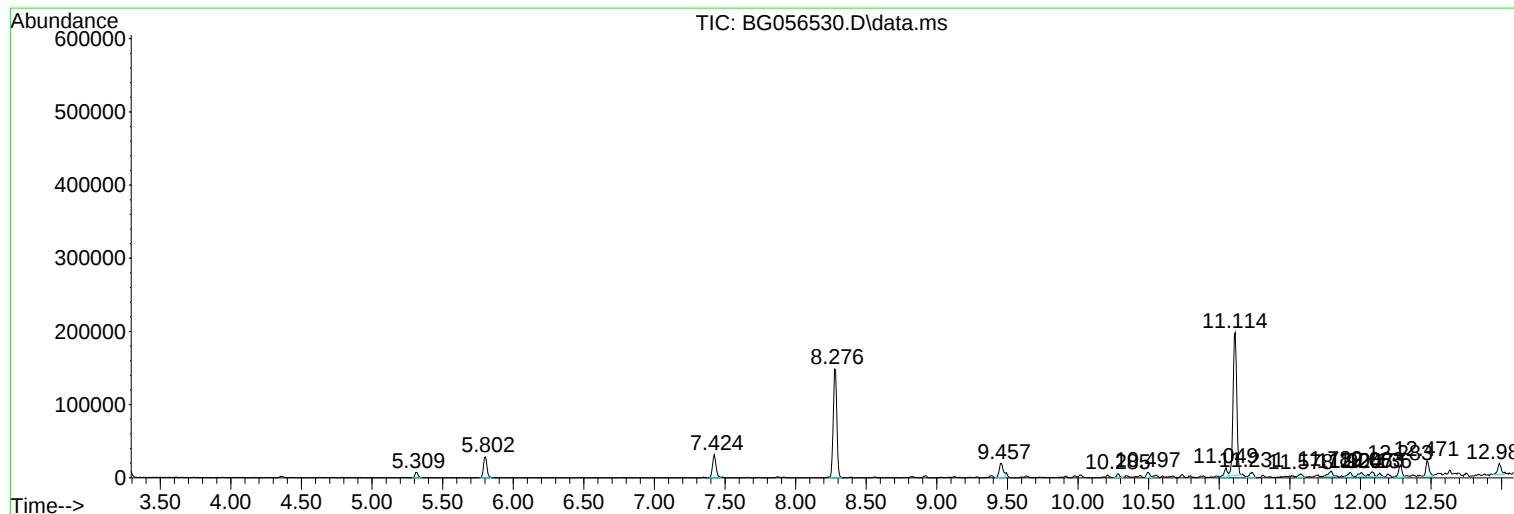
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Instrument :
BNA_G
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OK-1-212023

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG012723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG020223\
Data File : BG056530.D
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Operator : CG/JU
Sample : 01401-01 10X
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ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
OK-1-212023

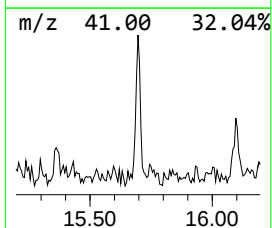
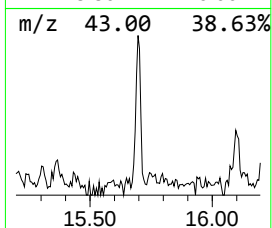
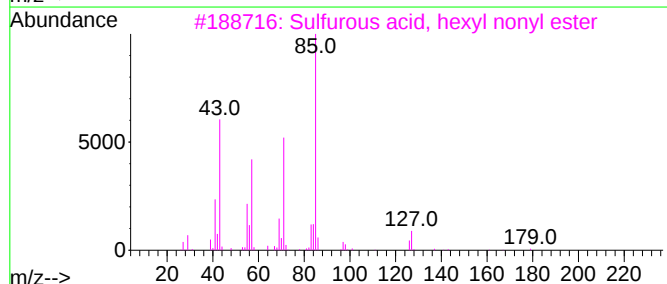
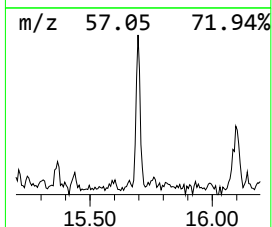
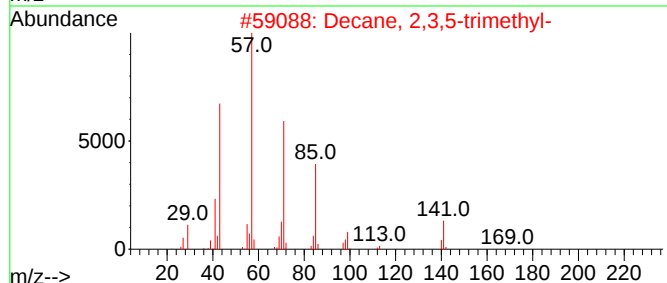
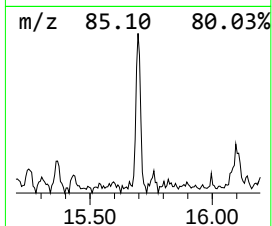
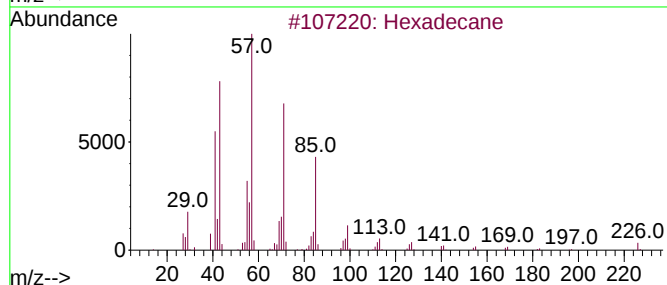
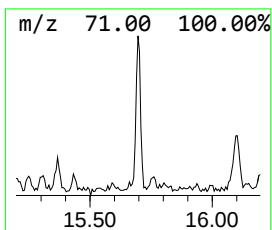
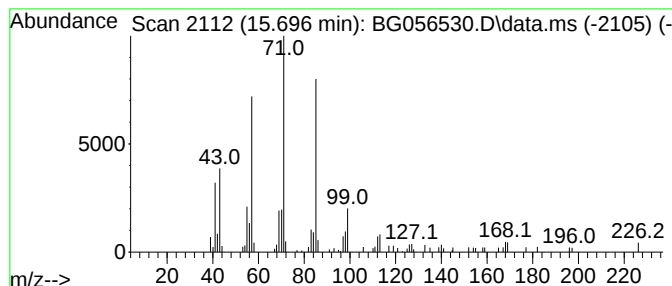
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG012723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Hexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.697	2.42 ng	65848	Acenaphthene-d10	14.897

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecane	226	C16H34	000544-76-3	90
2			Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	72
3			Sulfurous acid, hexyl nonyl ester	292	C15H32O3S	1000309-13-1	46
4			Sulfurous acid, hexyl tridecyl e...	348	C19H40O3S	1000309-13-5	38
5			Sulfurous acid, decyl hexyl ester	306	C16H34O3S	1000309-13-2	38



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Sample : 01401-01 10X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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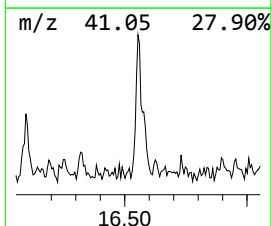
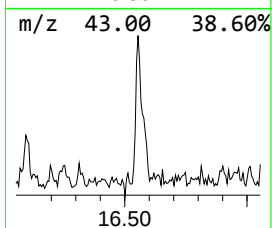
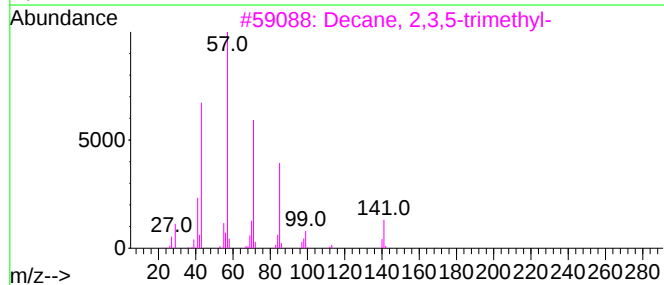
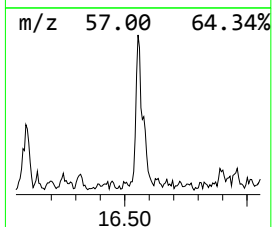
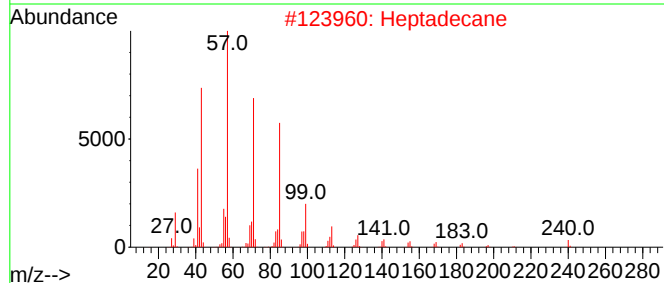
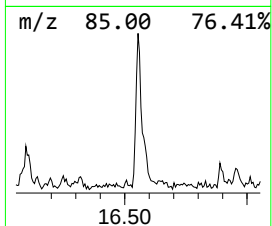
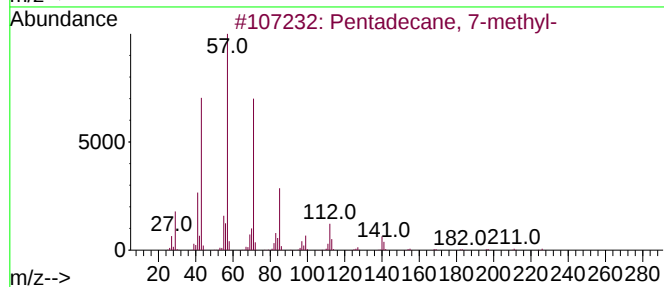
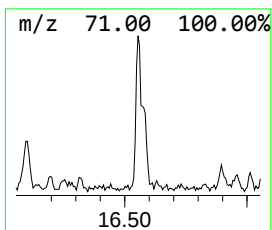
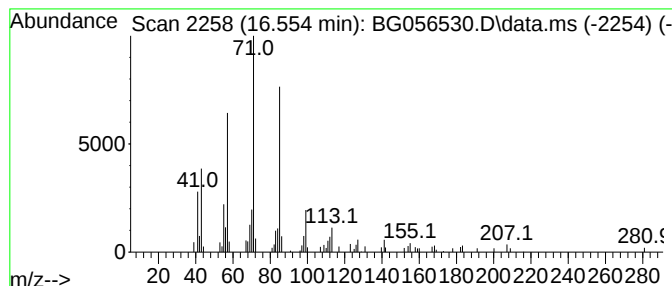
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG012723.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Pentadecane, 7-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.554	2.17 ng	71871	Phenanthrene-d10	17.635

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecane, 7-methyl-	226	C16H34	006165-40-8	86
2			Heptadecane	240	C17H36	000629-78-7	86
3			Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	86
4			Pentadecane	212	C15H32	000629-62-9	83
5			Hexacosane	366	C26H54	000630-01-3	83



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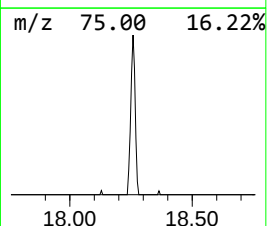
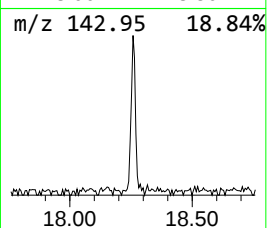
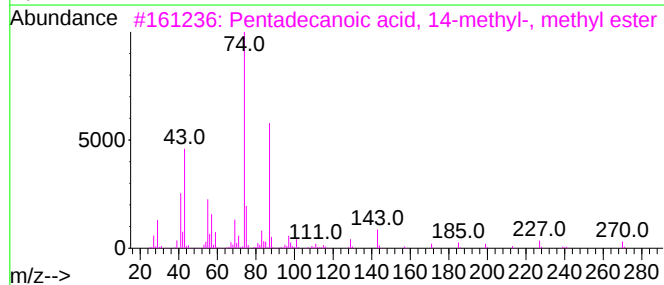
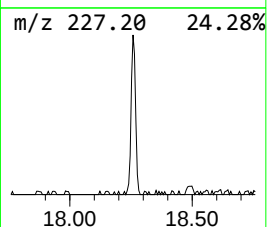
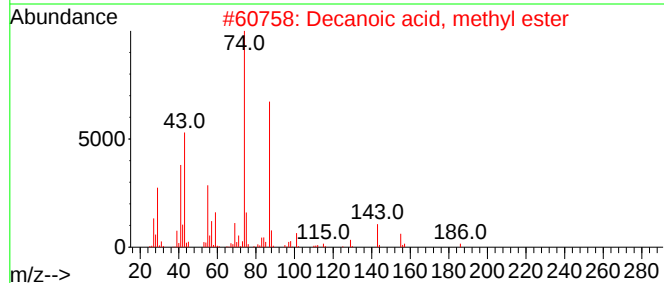
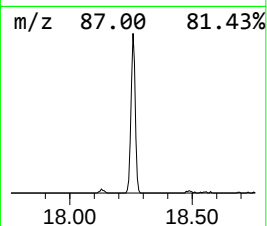
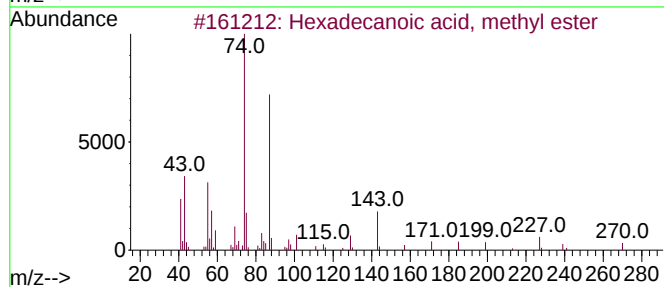
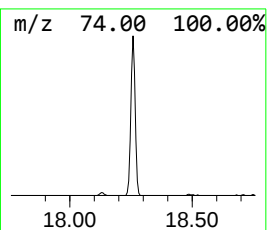
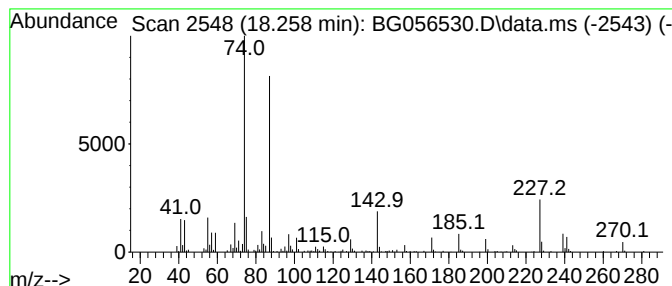
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG012723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Hexadecanoic acid, methyl e... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.258	7.47 ng	247487	Phenanthrene-d10	17.635

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	93
2			Decanoic acid, methyl ester	186	C11H22O2	000110-42-9	81
3			Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	81
4			Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	74
5			Methyl tetradecanoate	242	C15H30O2	000124-10-7	64



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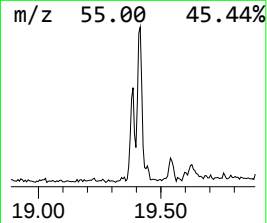
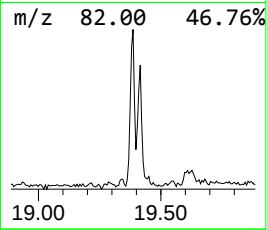
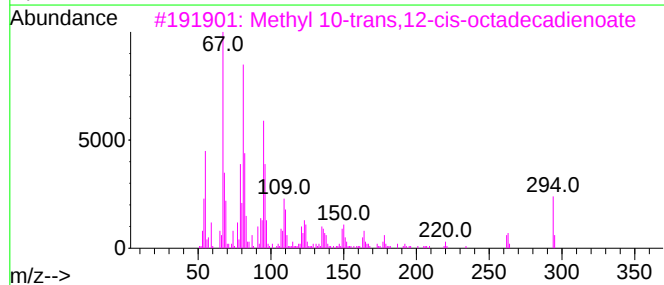
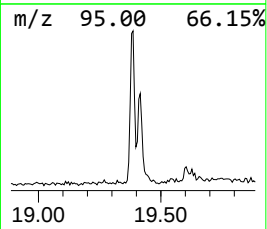
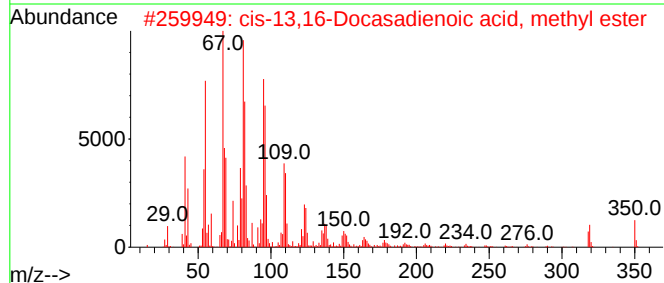
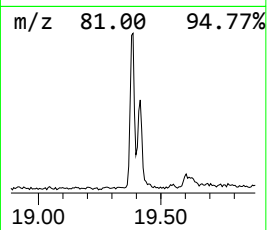
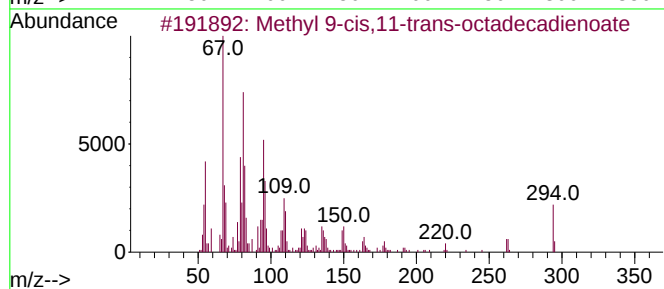
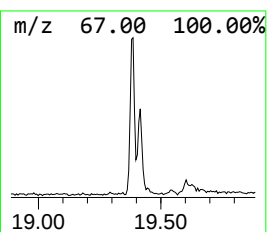
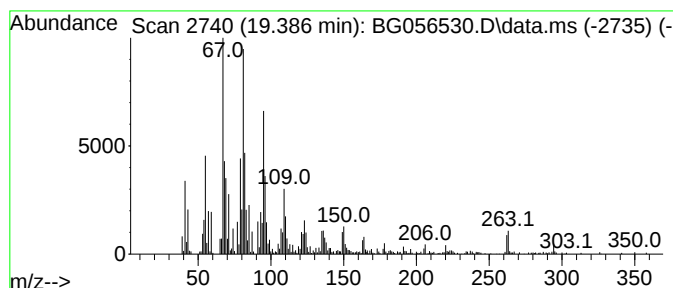
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Methyl 9-cis,11-trans-octad... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.386	13.46 ng	445907	Phenanthrene-d10	17.635

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl 9-cis,11-trans-octadecadi...	294	C19H34O2	013058-52-1	97
2			cis-13,16-Docosadienoic acid, me...	350	C23H42O2	1000333-60-3	96
3			Methyl 10-trans,12-cis-octadecad...	294	C19H34O2	1000336-44-2	93
4			9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	93
5			9,11-Octadecadienoic acid, methy...	294	C19H34O2	013038-47-6	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG020223\
Data File : BG056530.D
Acq On : 3 Feb 2023 1:41
Operator : CG/JU
Sample : 01401-01 10X
Misc :
ALS Vial : 15 Sample Multiplier: 1

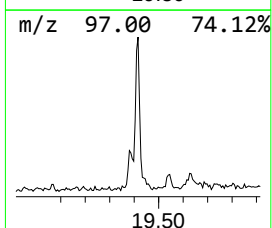
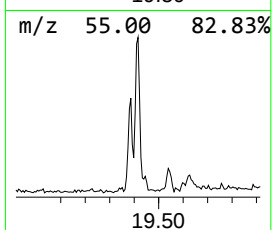
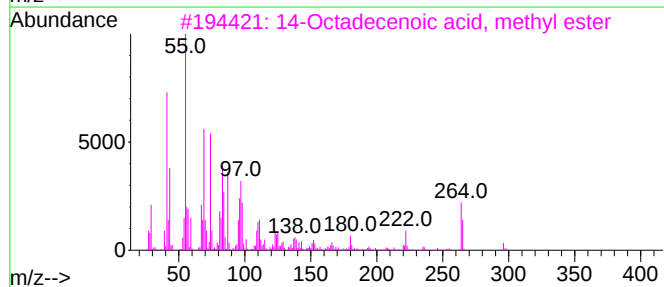
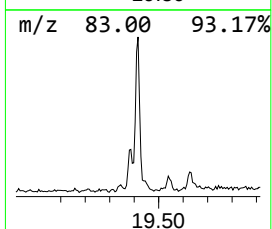
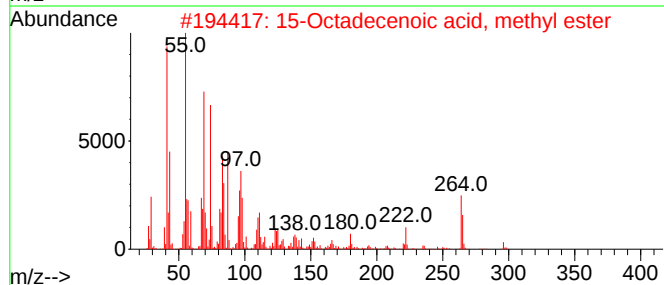
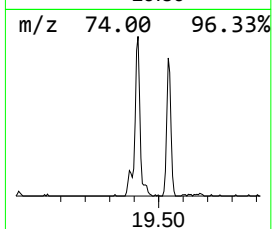
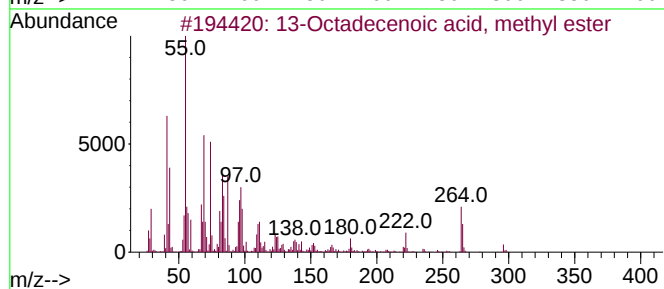
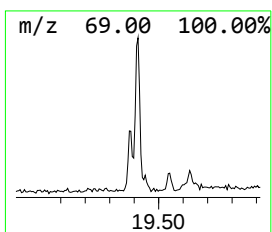
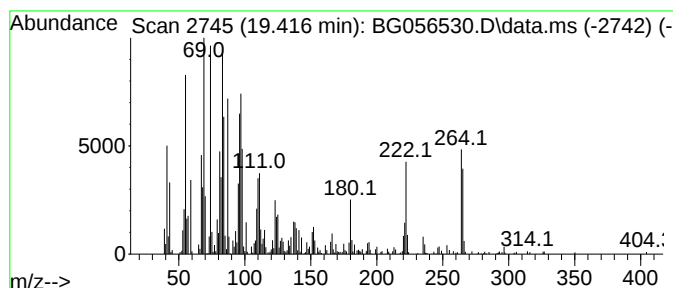
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ClientSampleId :
OK-1-212023

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 13-Octadecenoic acid, methyl... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD		R.T.	
19.416	16.62 ng	550583	Phenanthrene-d10		17.635	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	13-Octadecenoic acid, methyl ester		296	C19H36O2	056554-47-3	99
2	15-Octadecenoic acid, methyl ester		296	C19H36O2	004764-72-1	99
3	14-Octadecenoic acid, methyl ester		296	C19H36O2	056554-48-4	99
4	16-Octadecenoic acid, methyl ester		296	C19H36O2	056554-49-5	98
5	12-Octadecenoic acid, methyl ester		296	C19H36O2	056554-46-2	97



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG020223\
Data File : BG056530.D
Acq On : 3 Feb 2023 1:41
Operator : CG/JU
Sample : 01401-01 10X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
OK-1-212023

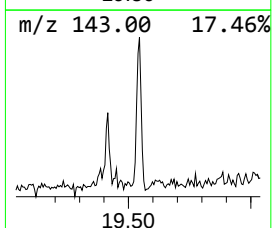
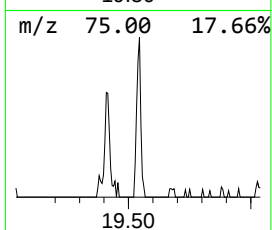
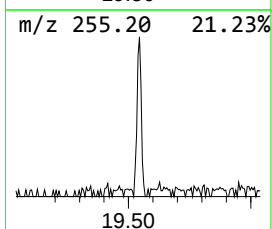
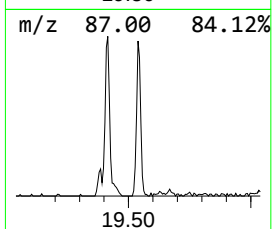
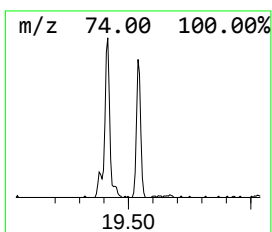
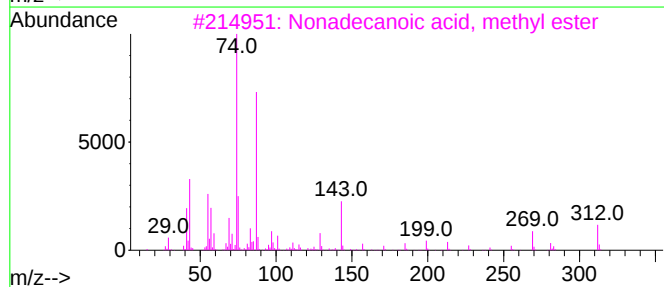
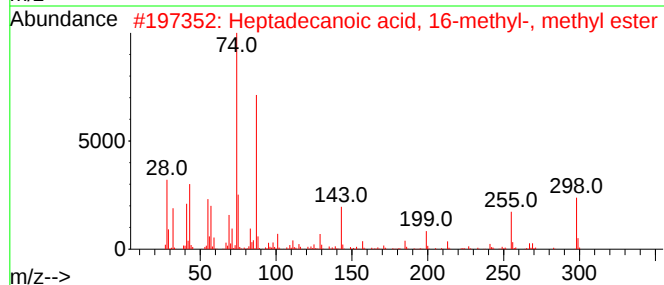
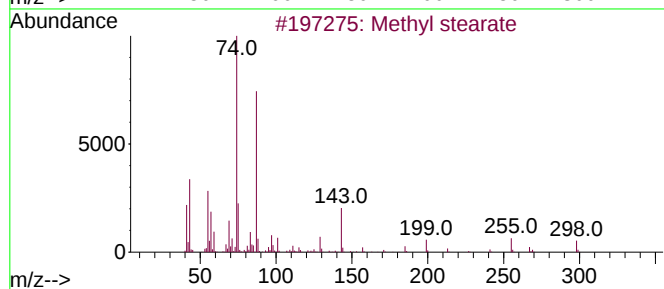
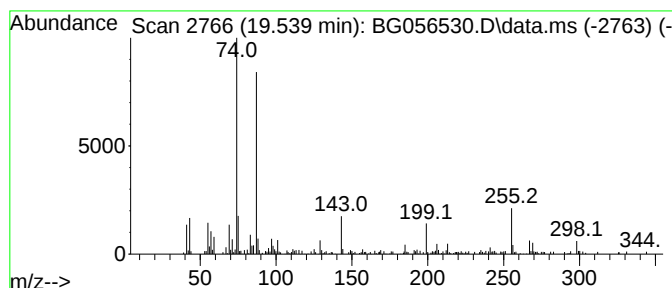
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Methyl stearate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.539	4.07 ng	134692	Phenanthrene-d10	17.635

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl stearate	298	C19H38O2	000112-61-8	91
2			Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	86
3			Nonadecanoic acid, methyl ester	312	C20H40O2	001731-94-8	83
4			Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	78
5			Methyl tetradecanoate	242	C15H30O2	000124-10-7	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG020223\
Data File : BG056530.D
Acq On : 3 Feb 2023 1:41
Operator : CG/JU
Sample : 01401-01 10X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
OK-1-212023

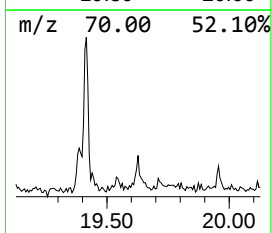
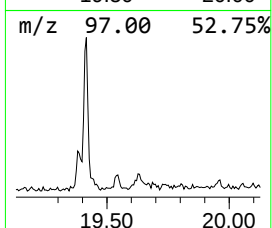
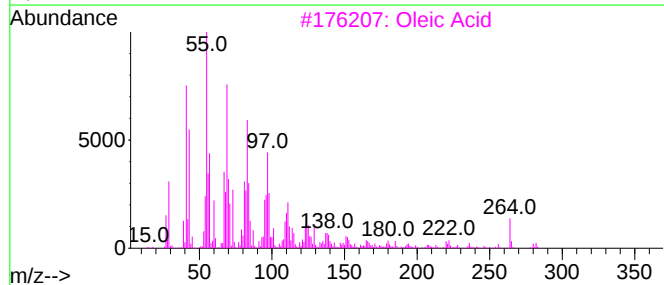
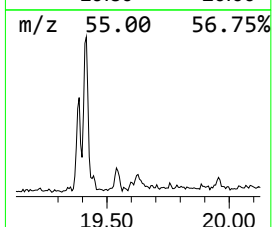
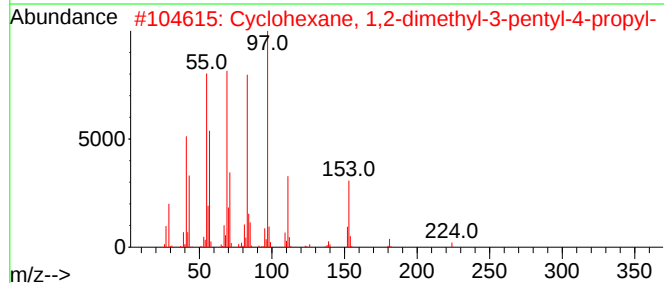
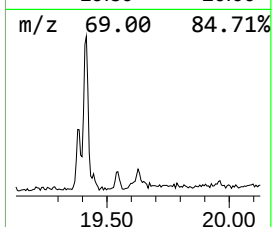
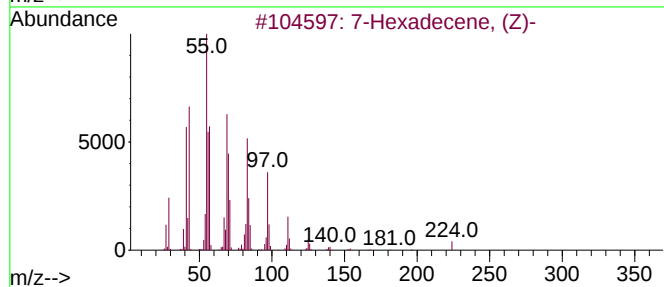
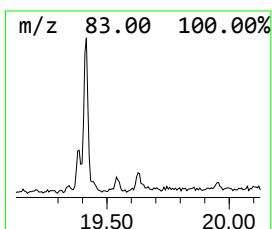
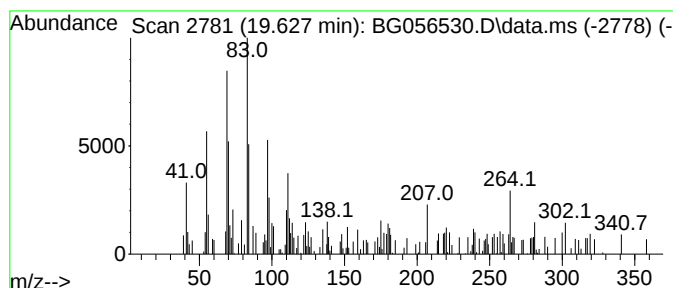
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 unknown19.627 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.627	2.00 ng	66264	Phenanthrene-d10	17.635

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7-Hexadecene, (Z)-	224	C16H32	035507-09-6	46	
2	Cyclohexane, 1,2-dimethyl-3-pent...	224	C16H32	062376-17-4	46	
3	Oleic Acid	282	C18H34O2	000112-80-1	43	
4	Cyclopropane, 1,1,2-trimethyl-3-...	140	C10H20	041977-43-9	38	
5	4-Undecene, 4-methyl-, (Z)-	168	C12H24	074630-57-2	38	



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG020223\
Data File : BG056530.D
Acq On : 3 Feb 2023 1:41
Operator : CG/JU
Sample : 01401-01 10X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
OK-1-212023

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG012723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Hexadecane	15.697	2.4	ng	65848	3	14.897	544403	20.0
Pentadecane, 7-...	16.554	2.2	ng	71871	4	17.635	662558	20.0
Hexadecanoic ac...	18.258	7.5	ng	247487	4	17.635	662558	20.0
Methyl 9-cis,11...	19.386	13.5	ng	445907	4	17.635	662558	20.0
13-Octadecenoic...	19.416	16.6	ng	550583	4	17.635	662558	20.0
Methyl stearate	19.539	4.1	ng	134692	4	17.635	662558	20.0
unknown19.627	19.627	2.0	ng	66264	4	17.635	662558	20.0